Anisole 100-66-3 | DTXSID4041608

Model Performance

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Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 2.42

Global applicability domain: Inside

Local applicability domain index: 6.30e-01

Confidence level: 7.90e-01

Nearest Neighbors from the Training Set

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Benzene, ethoxy-Measured: 2.51 Predicted: 2.48

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1-Methoxy-4-methylbenzene

Measured: 2.66 **Predicted:** 2.47

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3-Methoxytoluene Measured: 2.66 Predicted: 2.47

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Anisole
Measured: 2.11
Predicted: 2.42

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2-Fluoroanisole Measured: 2.14 Predicted: 2.56